

Breakdown of the power-law decay prediction of the heat current correlation in one-dimensional momentum conserving lattices

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We show that the asymmetric inter-particle interactions can induce rapid decay of the heat current correlation in one-dimensional momentum conserving lattices. When the asymmetry degree is appropriate, even exponential decay may arise. This fact suggests that the power-law decay predicted by the hydrodynamics may not be applied to the lattices with asymmetric inter-particle interactions, and as a result, the Green-Kubo formula may instead lead to a convergent heat conductivity in the thermodynamic limit. The mechanism of the rapid decay is traced back to the fact that the heat current has to drive a mass current additionally in the presence of the asymmetric inter-particle interactions.

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Onsager's classic work [1] has shown that in the linear response region, the current J_i of a physical quantity can be expanded in terms of the so-called thermodynamic forces, i.e., $J_i = \sum_j \kappa_{ij} F_j$. The Onsager coefficient κ_{ij} , which describes the coupling between the forces F_i and F_j , can be calculated in terms of the correlation function of the spontaneous current fluctuations as [2],

$$\kappa_{ij} = \lim_{\tau \rightarrow \infty} \lim_{L \rightarrow \infty} \frac{1}{2} \int_0^\tau C_{ij}(t) dt, \quad (1)$$

where $C_{ij}(t) \equiv \langle (J_i(t) - \langle J_i \rangle)(J_j(0) - \langle J_j \rangle) \rangle$ and L is the linear dimension of the system along which the current flows. The celebrated Onsager reciprocal relation formulates the relation between the coupling coefficients, which gives $\kappa_{ij} = \kappa_{ji}$. However, we recall that under what condition the coupling coefficients are non-vanishing, and what a role the couplings may play in characterizing the transport process, have not been clarified.

Equation (1) is the well-known Green-Kubo formula. It provides a way for calculating the transport coefficient by considering the current fluctuations in equilibrium state. The traditional hydrodynamic approach assumed that the current correlation decays rapidly, i.e., exponentially fast, so to ensure the convergence of the integral in the Green-kubo formula [3, 4]. However, after Alder numerically evidenced the 'long time tail' of the correlation function of the energy current in 1970 [5] in a gas model, a lot of theoretical analysis as well as numerical simulations have shown that the autocorrelation functions of currents in one-dimensional (1D) fluids may generally decay in a power-law manner instead [6–8]. The power-law decay is explained within the framework of hydrodynamics, where the slow diffusion of long wave hydrodynamic modes or the ring-collision of particles are ascribed to be the underlying mechanisms.

In recent decades, low-dimensional materials such as nanowires and graphene flakes have come into focus in many disciplines. The studies of them are undergoing rapid progress for both fundamental research interests

and various intriguing applications. The heat transport properties of low-dimensional lattice models have been a particularly interesting issue. An important progress is that the hydrodynamic analysis has been extended to the study of the transport behavior in lattices. Based on intensive theoretical analysis [4, 9–14] and numerical studies (see for example [7, 8] and references there in), for 1D momentum conserving fluids and lattices, at present it is generally believed that the current correlation should decay in the power-law manner. An important consequence of the power-law decay is that the integral in the Green-Kubo formula will diverge. For a finite system size, to truncate the integration at a reasonable time may lead to a finite transport coefficient, but, however, it may diverge in the thermodynamical limit in a way of $\kappa_{ij} \sim L^\nu$ (with $\nu > 0$).

Meanwhile, several counterexamples to the divergent heat conductivity have also been reported, including the rotator model [16], a 1D lattice in an effective magnetic field [17], the variant ding-a-ling model [18], and lattice models with asymmetric inter-particle interactions [19]. We notice that in the counterexamples studied in Ref. [18] and [19], asymmetric inter-particle interactions are quite relevant. Hence a natural question is what effect the asymmetric interactions may have on the 'long time tail' decay and result in a finite, convergent heat conductivity. In fact, lattice models with asymmetric interactions have been studied in the literature, both analytically [9, 10, 14] and numerically [10, 24]. In particular, the hydrodynamic analysis based on the Burgers equation suggests that $\alpha = 1/2$ for systems with asymmetric interactions and $\alpha = 1/3$ for those with only symmetric interactions [9], which agrees with the result based on the Zwanzig-Mori equation and the self-consistent mode coupling theory [14].

In this paper, by employing two paradigmatic lattice models, the Fermi-Pasta-Ulam- α - β (FPU- α - β) model and the Lennard-Jones (L-J) model, we show that the power-law decay of the current correlation may vanish

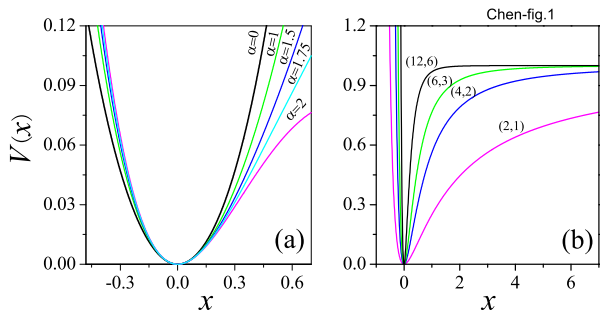


FIG. 1: Plots of the inter-particle potentials investigated: The potential of (a) the FPU- α - β lattice model and (b) the L-J lattice model.

in the presence of the asymmetric interactions. Instead, rapid decay fast than the power law is observed in both models. It is well known that systems with symmetric and asymmetric interactions have remarkable different properties. For example, the thermal expansion effect is exclusive in the latter. In the following, we shall conjecture that the thermal expansion effect is also responsible for the rapid decay of current correlation functions. For this aim we have to confront the previous numerical results in the literature and the contradictory hydrodynamic predictions. On one hand, we shall provide careful, large-scale simulation results, and show the importance to keep the lattice features of the models in the simulations and the sensitive dependence of the results on the asymmetry degree. As to the hydrodynamic predictions, we think it is still open. As the hydrodynamic analysis is based on the linearized hydrodynamic equations, one possibility is that the role of the asymmetric interactions may not have been sufficiently considered if their main effects are contained in the high order terms. We shall show that the energy current can excite the mass current in systems with asymmetric interactions, while there lacks such a coupling between the energy and the mass current in systems of symmetric interactions. We shall also illustrate that, different from the fluid models, the lattice structure can additionally scatter the currents. These facts are crucial for the rapid decay of current correlation but have not been involved explicitly in the previous hydrodynamic analysis.

Our models are defined by the Hamiltonian

$$H = \sum_i \frac{p_i^2}{2} + V(x_i - x_{i-1} - 1), \quad (2)$$

where p_i and x_i are the momentum and position of the i th particle, respectively, and V the potential between neighboring particles. The component particles are assumed to be identical and have unit mass, and the lattice constant is set to be unity so that the system length L equals the particle number N . The inter-particle interactions in

the FPU- α - β model is

$$V(x) = \frac{1}{2}x^2 - \frac{\alpha}{3}x^3 + \frac{1}{4}x^4, \quad (3)$$

where the parameter α controls the degree of asymmetry as illustrated in Fig. 1(a). For $\alpha = 0$ the system reduces to the Fermi-Pasta-Ulam- β (FPU- β) model with symmetric potential only. To well reveal the effects of the asymmetry, in our simulations the average energy per particle, denoted by ε , is fixed to be $\varepsilon = 0.1$ such that the averaged potential energy per particle is about 0.05.

The potential of the L-J model is

$$V(x) = \left[\left(\frac{1}{x+1} \right)^m - 2 \left(\frac{1}{x+1} \right)^n + 1 \right]. \quad (4)$$

This potential may well approximate the inter-particle interactions in many real materials, and hence has important practical implications. In this potential the degree of asymmetry is controlled by the parameter set (m, n) . (See Fig. 1(b) for several examples.) It should be noted that if the average potential per particle is larger than one then the potential models fluids instead. So in our simulations the average energy per particle is fixed to be $\varepsilon = 0.5$ to make sure that our model is a lattice. As shown in Fig. 1(b), the degree of asymmetry increases as (m, n) changes from $(12, 6)$ to $(6, 3)$, and to $(2, 1)$.

The energy current [21] is defined as $J_q \equiv \sum_i \dot{x}_i \frac{\partial V}{\partial x_i}$. For a lattice the energy current is equal to the heat current because there is no residual global velocity [7]. To numerically measure the current in the equilibrium state, the system is first evolved from an appropriately assigned random initial condition for a long enough time ($> 10^8$) to ensure that it has relaxed to the equilibrium state; then the current at ensuing times is measured. The periodic boundary condition is applied in the calculations.

Figure 2 shows the autocorrelation of the energy current $C_{J_q J_q}(t) \equiv \frac{\langle J_q(t) J_q(0) \rangle}{\langle J_q(0) J_q(0) \rangle}$ for the two models. The results are presented in semi-log scale in panel (a) and (c) and in log-log scale in panel (b) and (d). In generating Fig. 2, the system size is fixed to be $N = 2048$ which is sufficiently large because we have checked that the results does not change if the system size is increased further. It can be seen that in the FPU- α - β model which involves symmetric potential, the correlation function decays in a power law $C_{J_q J_q}(t) \sim t^{-\gamma}$ with $\gamma \sim 0.67$, which agrees well with previous studies [21]. Therefore, it provides an example that with the symmetric interactions, the long-time-tail prediction applies. However, for the FPU- α - β model with $\alpha > 1$, we can see that the decay become faster than the power-law manner which can be roughly regarded to be exponentially. For the L-J model, the decay is much close to a perfect exponential manner for different sets of control parameters (m, n) . With the increase of the asymmetry, the decay become faster and faster.

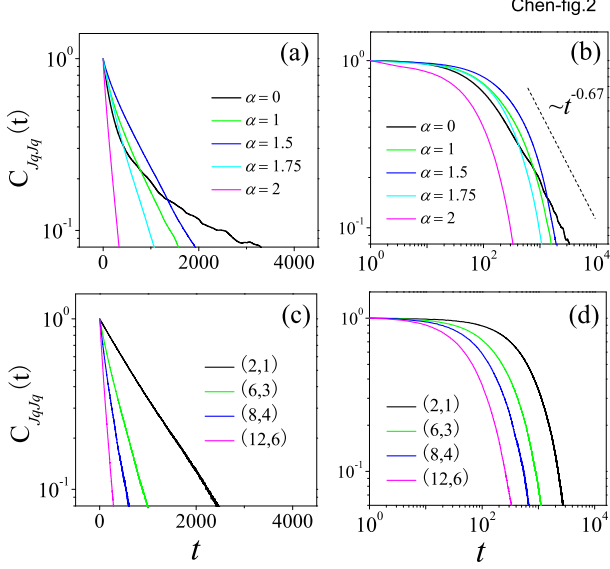


FIG. 2: The autocorrelation function of the heat flux. (a) and (b) are respectively the semi-log plot and log-log plot of FPU- α - β model; (c) and (d) are the same but for the L-J model.

The thermal expansion effect induced by the asymmetric interactions could be a key for understanding the mechanism [19]. Thermal expansion implies the coupling between the energy and mass distribution. Because of the coupling, redistribution of energy can induce redistribution of mass. In the following, we demonstrate that in equilibrium state, asymmetry interactions can do result in the coupling between the fluctuations of the energy current and the mass current. As the global mass current in equilibrium state is zero due to the fact that the total momentum of the system is zero, the cross correlation between the global energy and mass currents is zero as well. However, the local mass current of a part of the system, i.e., $J_m \equiv Mv$, may still fluctuate. Here M is the mass of the whole part of the system and v represents its center-of-mass velocity. We thus investigate the coupling between the local energy current and the local mass current. To be concrete, in the simulations we consider a quarter of the whole system as our local subsystem.

Figure 3(a) shows the cross correlation of the local energy current J_q and the mass current J_m as function of time for the FPU- α - β model with $\alpha = 2$. It can be seen that $\langle J_q(0)J_m(t) \rangle$ and $\langle J_m(t)J_q(0) \rangle$ perfectly agree with each other, suggesting that the Onsager reciprocal relation, $\kappa_{qm} = \kappa_{mq}$, holds even for the subsystem. In Fig. 3(b), the cross correlation at the same time, i.e., $\langle J_q(t)J_m(t) \rangle$, is shown as a function of the asymmetry parameter α . It can be seen that the cross correlation decreases with the decrease of the asymmetry. In particular, in the symmetric limit with $\alpha = 0$, the correlation

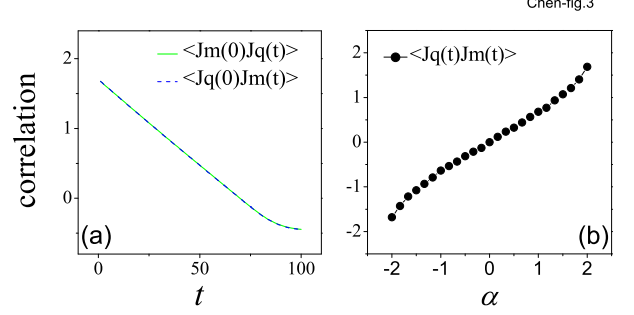


FIG. 3: (a) The cross correlation functions between the local heat flux J_q and the local mass flux J_m for the FPU- α - β model with $\alpha = 2$. (b) The dependence of the cross correlation function $\langle J_q(0)J_m(0) \rangle$ on the asymmetry parameter α .

vanishes, which reveals clearly that it is the asymmetry that sustains the coupling between the currents.

The fact that a symmetric potential leads to a vanishing cross current correlation can be shown analytically. In the continuum limit, the local energy current can be written as $j = \langle \dot{x} \frac{\partial V}{\partial x} \rangle$. In addition, the mass density is a scalar variable and satisfies $\rho(x) = \rho(-x)$ because the potential is symmetric and hence we have $V(x) = V(-x)$. Considering all of these, it is straightforward to derive that

$$\left\langle \int_{-l}^l \dot{x} \frac{\partial V(x)}{\partial x} \dot{x} \rho(x) dx \right\rangle = - \left\langle \int_{-l}^l \dot{x} \frac{\partial V(x)}{\partial x} \dot{x} \rho(x) dx \right\rangle,$$

which implies a zero cross correlation immediately. Here the integration is taken over the subsystem on which the local mass current is defined. Here $(-l, l)$ represents the lattice segment of the subsystem.

Therefore, in a system with the asymmetric interactions, once a fluctuation of energy current forms spontaneously, a mass density fluctuation will be excited. The resultant mass current is driven by the energy current due to their nonzero cross correlation, hence the mass current should serve as a resistant factor to the energy current.

This mechanism alone, however, can not explain the rapid decay of the current correlation. The conventional hydrodynamic theory has predicted that low-dimensional fluids should show slow-decay of current correlation. For the 1D diatomic gas previous simulations [22] have shown the power-law decay of $C_{qq}(t) \sim t^{-0.67}$. We have reformed the simulation and obtain the same result. In this model, particles interact via the hard-core collisions, which is the limit case of the asymmetry potential. This fact indicates that the lattice feature should also be crucial to the fast decay.

The spatiotemporal cross correlation of fluctuations of the local energy current and the local mass current may shed light on the role of the lattice feature. For this

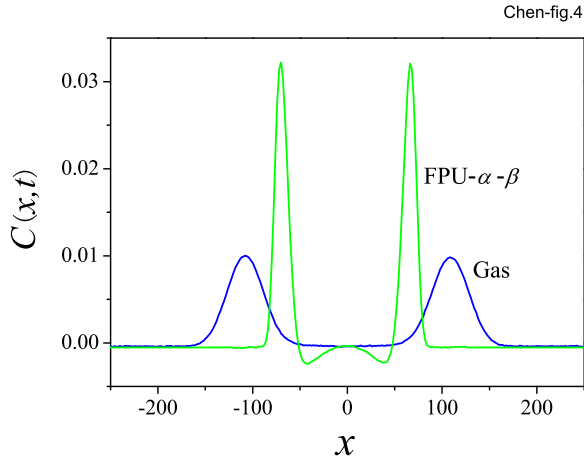


FIG. 4: The spatiotemporal cross correlation of fluctuations of the local energy current and mass current for (a) the FPU- α - β model (Green) and (b) the gas model (Blue).

purpose we divide the whole system into N equal bins. Then the global current J can be expressed as the sum of the local ones, i.e., $J = \sum_k j_k$, where j_k represents the local current of the k th bin. We use

$$C(x, t) = \langle j_k^q(0) j_l^m(t) \rangle \quad (5)$$

to measure the spatiotemporal cross correlation between the local energy current j_k^q in the k th bin at $t = 0$ and the local mass current j_l^m in the l th bin at time t , where $x \equiv (l - k)$. Figure 4 shows the results for the FPU- α - β model with $\alpha = 2$ and $\varepsilon = 0.1$ and the diatomic gas model with mass ratio $1/3$ and $\varepsilon = 1$. The difference is remarkable: In the lattice model the positive correlation peaks are followed by regions with negative correlation, while in the gas model there are only positive correlation peaks. These observations indicate that in the lattice model, as the mass current flows in one direction, a accompanying mass current in the reverse direction will be excited as well. Because of the coupling between the energy and mass current, it also implies that an energy current in the reverse direction is induced as well. In other words, the currents are reflected as they flow forwards, and a decay mechanism is thus resulted in. However, such a mechanism is absent in the gas model.

In summary, we have shown that the asymmetric inter-particle interactions could result in nonvanishing coupling between the local energy current and the local mass current, and the coupling coefficients follow the Onsager reciprocal relation. In the case of the symmetric interactions, the coupling vanishes. The asymmetric interactions can induce rapid decay of the current correlation in 1D momentum conserving lattices, and results in finite thermal conductivities in the thermodynamic limit. As the asymmetric interactions, signaled by the thermal

expansion effect [25], are common in real materials, this finding should have universal implications.

Our simulations indicate that even perfect exponential decay can be observed with appropriate degree of asymmetry. However, based on numerical studies with finite-size effects, at present it is difficult to conclude with certainty that the asymmetric interactions can *generally* lead to the faster than the power-law decay in the current correlation. The degree of asymmetry is not only determined by the control parameters but also depends on the temperature of the system. For example, at the same control parameter of $\alpha = 1$ we have observed fast decay of the current correlation in the FPU- α - β model, while in previous studies [24] a power-law like decay was observed. The difference roots in the temperature: in [24] a much higher temperature was investigated, hence the potential is in effect dominated by the quartic term and shows a more symmetric structure. To clarify in detail the dependence of the decay behavior of current correlation on the degree of asymmetry should be a task for next studies.

Another more challenging task for future studies is to answer why the direct simulation results as presented here disagree with certain hydrodynamic predictions. One clue we provide in this paper is that the coupling effect between the heat and the mass current. With the asymmetric interactions, local heat currents may excite local mass currents, hence the latter may be an resistant factor to the former. In the case of symmetric interactions, the coupling effect vanishes. On the other hand, the currents can also be scattered by the lattice structure in the presence of asymmetric interactions. This mechanism is absent in the fluid model we studied. This observation may explain why in the one-dimensional diatomic gas a power-law decay can be observed though the inter-particle interactions are also asymmetric.

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